



Algebraic Solvers in FASTMath

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Part 1 – Introduction to several packages unable to present today
Part 2 – Portable Extensible Toolkit for Scientific computing



■ Capabilities:

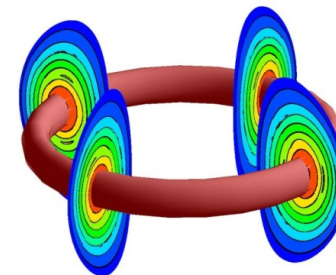
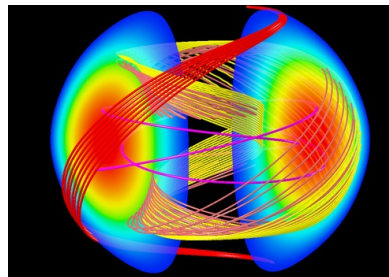
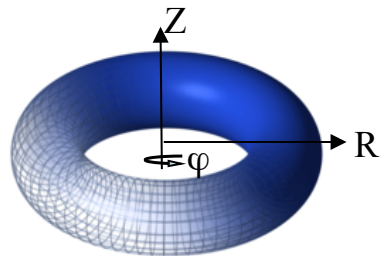
- Serial (C), shared-memory (Pthreads or OpenMP, distributed-memory in MPI; with Fortran interface.
- Sparse LU decomposition, triangular solution with multiple right-hand sides
- Incomplete LU (ILU) preconditioner (serial SuperLU)
- Sparsity-preserving ordering
 - Minimum degree ordering applied to $A^T A$ or $A^T + A$ [MMD, Liu '85]
 - ‘Nested-dissection’ applied to $A^T A$ or $A^T + A$ [(Par)Metis, (PT)-Scotch]
- User-controllable pivoting: partial pivoting, threshold pivoting, static pivoting
- Condition number estimation
- Iterative refinement
- Componentwise error bounds

■ Download: www.crd.lbl.gov/~xiaoye/SuperLU

■ Further information: contact: Sherry Li, xsli@lbl.gov

- Developers: Sherry Li, Jim Demmel, John Gilbert, Laura Grigori, Meiyue Shao, Ichitaro Yamazaki

- A new fusion reactor ITER is being constructed in France, which is used to study how to harness fusion, creating clean energy using nearly inexhaustible hydrogen as the fuel. If successful, ITER will produce 10 times as much energy than it uses — but that success hinges on accurately designing the device.
- One major simulation goal is to predict microscopic MHD instabilities of burning plasma in ITER. This involves solving extended and nonlinear Magnetohydrodynamics equations. Two fluid-based codes have been developed, using different finite element discretization methods: M3D-C1 (Steve Jardin et al. PPPL), and NIMROD (Carl Sovinec, Univ. Wisconsin, and others)
- These are truly multiphysics simulations involving several coupled PDEs: continuity, Maxwell, momentum, electron energy, ion energy, etc. They are also of multiscale with extremely wide range of time and spatial scales, and high anisotropy. Therefore, the discretized linear systems are indefinite and very ill-conditioned.
- SuperLU_DIST has been used in the production codes. For example, the NIMROD simulation time was **improved from 3 weeks to 3 days**, compared to using some preconditioned iterative solvers. In many iterations of nonlinear solver, the largest linear systems are of dimension 500K, complex and nonsymmetric.



- There were over 24,000 downloads of SuperLU in FY 2012.
 - It was the third most-downloaded software at LBNL
 - Over the years, it has consistently been the most-downloaded software in the Computing Sciences organization at LBNL
- It has been used in many high-end simulation codes, such as ASCEM (reactive flow and transport), M3D-C¹/NIMROD (fusion tokamak design), Omega3P (accelerator cavity design), OpenSees (earthquake engineering), PHOENIX (modeling of stellar and planetary atmospheres).
- It is adopted in many commercial mathematical libraries and simulation software, including AMD (circuit simulation), Boeing (aircraft design), Chevron (geology), Cray's LibSci, FEMLAB, HP's MathLib, IMSL, NAG, OptimaNumerics, Python (SciPy), Walt Disney Feature Animation.

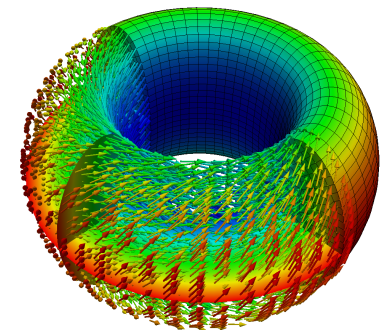
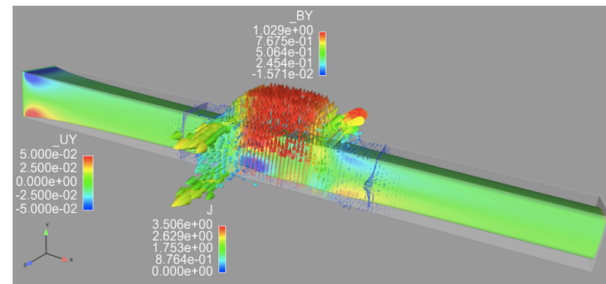
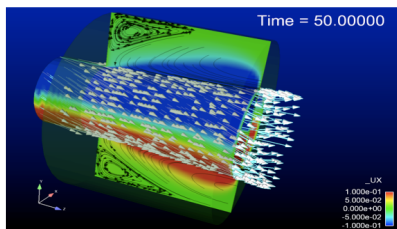
■ Capabilities:

- Algebraic multigrid (AMG) algorithms
 - Smoothed aggregation AMG (Poisson, elasticity)
 - Petrov Galerkin AMG (convection-diffusion)
 - H(curl) AMG (electro-magnetic)
- Coarsening algorithms
 - Uncoupled, MIS, METIS, ParMETIS
- Smoothers
 - Jacobi, (symmetric) Gauss-Seidel, polynomial (Chebyshev), ILU, block variants, user-provided

■ **Download:** trilinos.sandia.gov/download

■ **Further information:** trilinos.sandia.gov/packages/ml

- Drekar simulation software
 - low mach incompressible Navier Stokes
 - Magneto-hydrodynamics
- Drekar makes extensive use of Trilinos framework:
 - Panzer, Phalanx, Intrepid, ML, Ifpack, Amesos, Zoltan, AztecOO
- Simulations have been run on up to 512K Bluegene/Q cores and 128K cores of Titan.



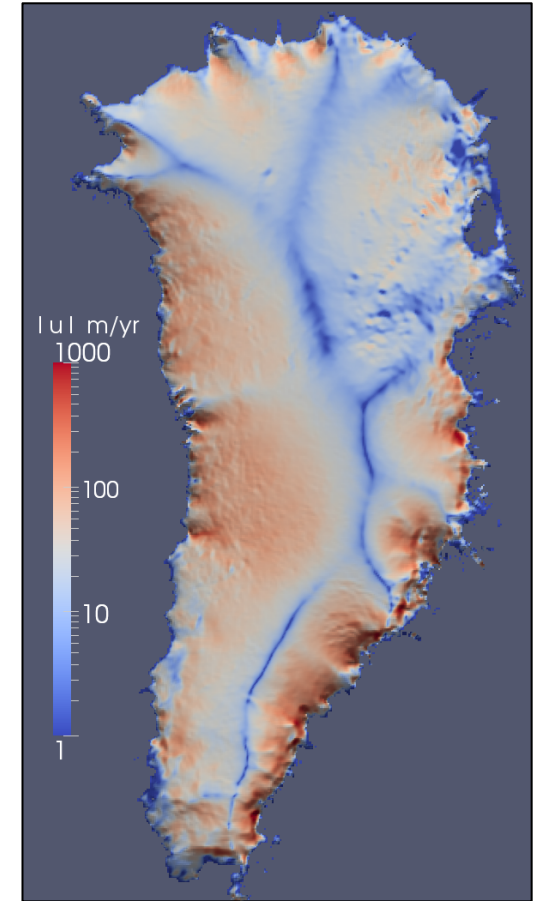
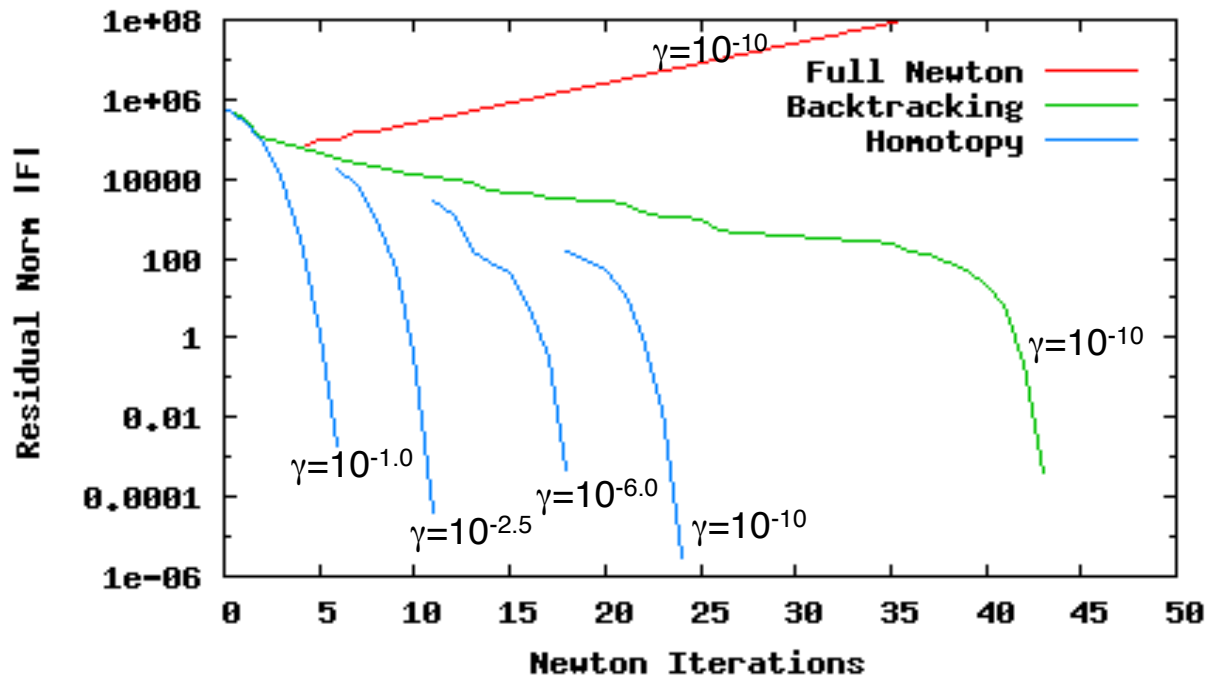
■ Capabilities:

- Newton-Based Nonlinear Solver
 - Linked to Trilinos linear solvers for scalability
 - Matrix-Free option
- Globalizations for improved robustness
 - Line Searches, Trust Region, Homotopy methods
- Customizable: C++ abstractions at every level
- Extended by LOCA package
 - Parameter continuation, Stability analysis, Bifurcation tracking

■ Download: Part of Trilinos (trilinos.sandia.gov)

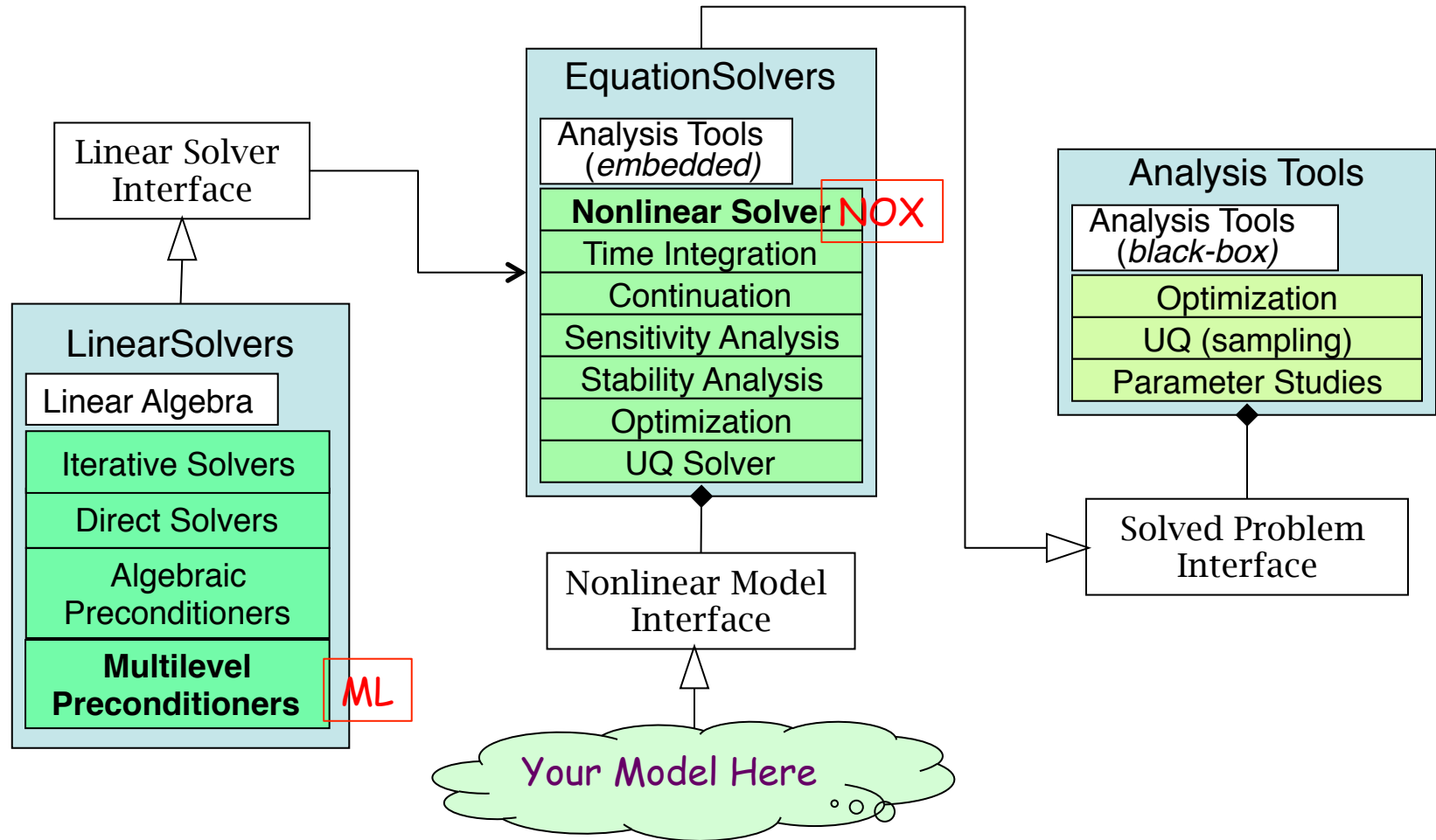
■ Further information: Andy Salinger [agsalin@sandia.gov]

- Ice Sheets modeled by nonlinear Stokes's equation
 - Initial solve is fragile: Full Newton fails
 - Homotopy continuation on regularization parameter " γ " saves the day



Greenland Ice Sheet
Surface Velocities
(constant friction model)

NOX and ML are part of larger Trilinos solver stack: Linear solvers, Equations solvers, Analysis tools



■ Capabilities:

- Compute a few eigenpairs of a Hermitian and non-Hermitian matrix
- Both standard and generalized eigenvalues
- Extremal and interior eigenvalues
- Reverse communication allows easy integration with application
- MPI/BLACS communication

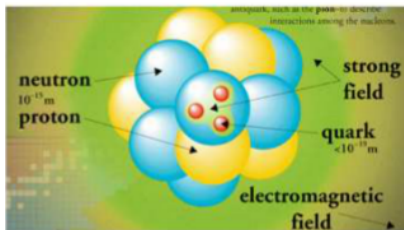
■ Download:

<http://www.caam.rice.edu/software/ARPACK/>

■ Further information: beyond PARPACK

- EIGPEN (based on penalty trace minimization for computing many eigenpairs)
- Parallel multiple shift-invert interface for computing many eigenpairs

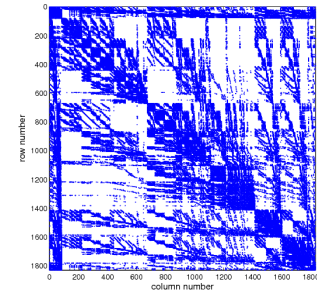
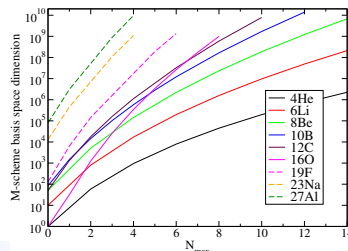
- MFDn (Many-body Fermion Dynamics for nuclear physics) is the most robust and efficient configuration interaction code for studying nuclear structure
- Solve the nuclear quantum many-body problem



$$\hat{H} \Psi(r_1, \dots, r_A) = \lambda \Psi(r_1, \dots, r_A)$$

$$\hat{H} = \frac{m}{2A} \sum_{i < j} (\vec{v}_i - \vec{v}_j)^2 + \sum_{i < j} V_{ij} + \sum_{i < j < k} V_{ijk} + \dots$$

- PARPACK allows low excitation states to be extracted from a low dimensional Krylov subspace



- A list of drivers provided in \$ARPACKTOPDIR/
PARPACK/EXAMPLES
- Reverse communication interface

```
10 continue
   call pdsaupd(comm, ido,...)
   if (ido .eq. 1 .or. -1) then
       matvec(...,workd(ipntr(1)), workd(ipntr(2))...
   endif
   goto 10
```

- Hybrid MPI/OpenMP implementation
- MATLAB interface available (eigs)